The Fascination of Crystals and Symmetry

Unit 2.6

by Frank Hoffmann & Michael Sartor
Fractional Coordinates

- Atom sites: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple \((x, y, z)\) and are fractional amounts of the lattice constants \((a, b, c)\)

\[
\begin{align*}
a &= 5 \text{ Å}, & b &= 20 \text{ Å}, & c &= 15 \text{ Å} \\
\alpha &= \beta = \gamma = 90^\circ \\
\end{align*}
\]

Atom 1: \(x = 2.5 \text{ Å}, y = 10 \text{ Å}, z = 7.5 \text{ Å} \quad \text{absolute coordinates}

Atom 1: \(0.5, 0.5, 0.5 \quad \text{relative or fractional coordinates}\)
Atom sites: Where are the atoms located inside of the unit cell?

- usage of the crystallographic system of coordinates
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- the atomic site parameters are given as a coordination triple \((x, y, z)\) and are fractional amounts of the lattice constants \((a, b, c)\)

**Example**

\(a = 5 \text{ Å}, b = 20 \text{ Å}, c = 15 \text{ Å} \quad \alpha = \beta = \gamma = 90^\circ\)

Atom 2: \(x = 5 \text{ Å}, y = 10 \text{ Å}, z = 0 \text{ Å}\) → absolute coordinates

Atom 2: \(1, 0.5, 0\) → relative or fractional coordinates
Fractional Coordinates

- **Atom sites**: Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple (x, y, z) and are fractional amounts of the lattice constants (a, b, c)

\[
a = 5 \, \text{Å}, \quad b = 20 \, \text{Å}, \quad c = 15 \, \text{Å} \quad \alpha = \beta = \gamma = 90^\circ
\]

Atom 3: \( x = 2.5 \, \text{Å}, \quad y = 20 \, \text{Å}, \quad z = 7.5 \, \text{Å} \) → absolute coordinates

Atom 3: \( 0.5, 1, 0.5 \) → relative or fractional coordinates
**Fractional Coordinates**

- **Atom sites:** Where are the atoms located inside of the unit cell?
  - usage of the crystallographic system of coordinates
  - the lattice constants are used as units
  - the atomic site parameters are given as a coordination triple \((x, y, z)\) and are fractional amounts of the lattice constants \((a, b, c)\)

\[
\begin{align*}
(0,0,0) &= (1,0,0) = (0,1,0) = \\
(1/2,0,1/2) &= \frac{1}{2}(1,0,0) = \frac{1}{2}(0,1,0) = \\
(1,1,1) &= (2,0,0) = (0,2,0) = \\
(1/2,1,1) &= \frac{1}{2}(2,0,0) = \frac{1}{2}(0,2,0) = \\
(0,1,1/2) &= (0,2,0) = (0,1,0) = \\
(1/2,1/2,1) &= \frac{1}{2}(2,0,0) = \frac{1}{2}(0,2,0) = \\
(1/2,0,1/2) &= \frac{1}{2}(1,0,0) = \frac{1}{2}(0,1,0) = \\
(0,1,1/2) &= (0,2,0) = (0,1,0) = \\
(1/2,1/2,1/2) &= \frac{1}{2}(2,0,0) = \frac{1}{2}(0,2,0) = \\
(1,1,1/2) &= (2,0,0) = (0,2,0) = \\
\end{align*}
\]
Fractional Coordinates – CuSO$_4$ · 5 H$_2$O

Chalcanthite

Space-group $P\overline{1}$
triclinic
$a = 5.9553$ Å
$b = 6.1084$ Å
$c = 10.7048$ Å

$\alpha = 77.4090^\circ$
$\beta = 82.3720^\circ$
$\gamma = 72.6740^\circ$

<table>
<thead>
<tr>
<th>Atomic parameters (x/a y/b z/c)</th>
</tr>
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<tbody>
<tr>
<td>Cu1 1/2 1/2 1/2</td>
</tr>
<tr>
<td>Cu2 1/2 0 0</td>
</tr>
<tr>
<td>S1 0.12527 -0.01315 0.28634</td>
</tr>
<tr>
<td>O1 0.64893 -0.28899 0.11748</td>
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<td>O2 0.65182 0.18247 0.07346</td>
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<td>O3 1.12844 -0.43479 0.12435</td>
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<td>O7 0.29749 -0.24436 0.31756</td>
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<td>O8 0.17223 0.09305 0.15153</td>
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<tr>
<td>O9 0.48076 0.75491 0.58387</td>
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</tbody>
</table>

Crystallographic Information File

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